ASCR Applied Mathematics Research Program: *Strategic Planning Activities*

David Brown

Presentation to ASCR Advisory Committee

Gaithersburg, MD

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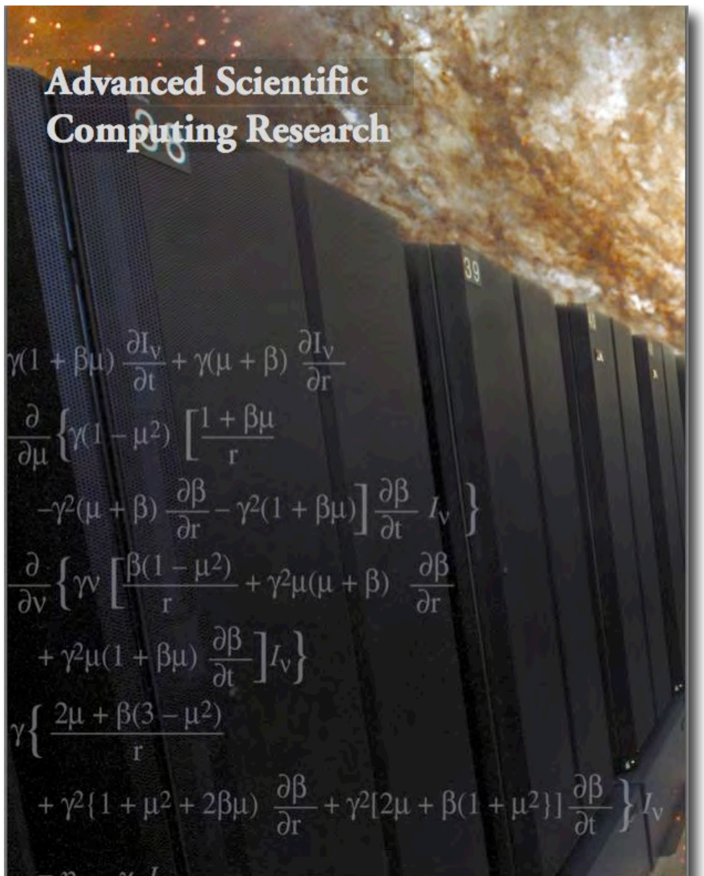
ASCR has an impressive 50 year legacy in applied and computational math -- what's next?

- Sustained support of world-class math PI's has resulted in models, analysis and algorithms for PDE-based science
  - Theory and numerical simulation of partial differential equations
  - Computational Fluid Dynamics
  - Scalable methods for solving large systems of linear and nonlinear equations
  - Methods for handling complex geometries, problems with sharp fronts, complex chemistry
  - Optimization methods
  - Mathematics of multiscale problems

John von Neumann suggested the creation of the AEC *applied math research* program in the early 1950's

ASCR will develop a strategic plan for math



- What applied and computational mathematics will be needed to address the challenges that the DOE faces over the next 50 years?

- ASCR must develop a strategic vision and plan that identifies critical enabling mathematics research areas for DOE

A panel of math experts met to discuss DOE challenges in applied mathematics


Donald Estep
CSU


Sallie Keller-McNulty
Rice

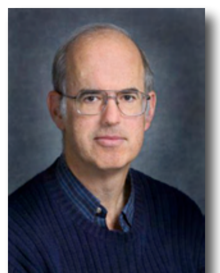

David Keyes
Columbia


Tinsley Oden
UTA


Linda Petzold
UCSB


Margaret Wright
NYU

- Recognized leaders in mathematics, statistics and computer science communities
- Broad background in applied mathematics topics
- Academic and lab representation
- Significant background with DOE and/or the Labs


John Bell
LBL


David Brown
LLNL (chair)


Bill Gropp
UIUC


Bruce Hendrickson
Sandia

Panel Meeting: August 23-24, 2007
Lawrence Berkeley National Laboratory

What scientific questions must DOE answer to accomplish its mission?

- Considered documents:
  - *DOE Strategic plan*
  - *DOE Program office Strategic plans & other documents*
  - *Energy Policy Act 2005 Report to Congress*
- Each panel member presented information from one office
- Together we extracted mathematical challenges for DOE

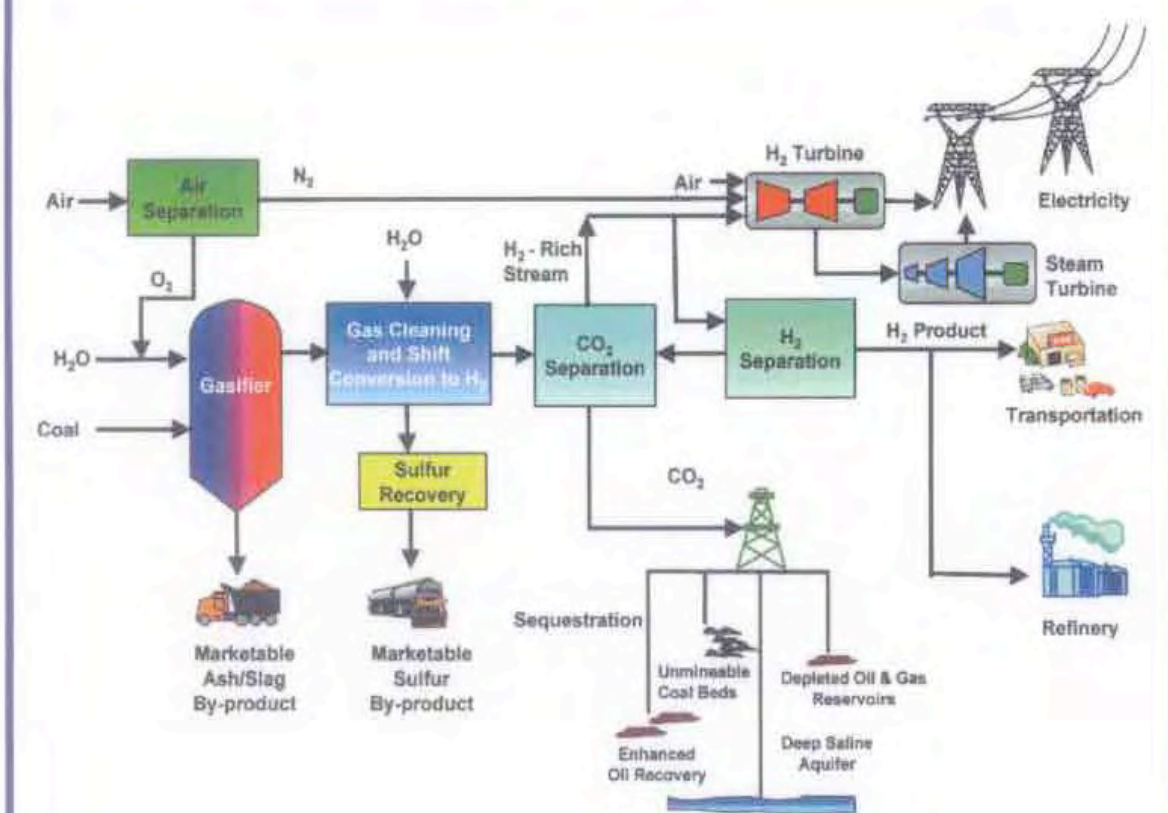
DOE must understand complex systems that arise across its mission space

- *Energy*
  - Nuclear power, clean coal, fusion reactors, enhanced oil recovery, bio-fuels, reliability & security of electric power grid, new engine designs
- *Environment*
  - Carbon sequestration, nuclear waste storage, environmental cleanup, climate modeling
- *National Security*
  - Nuclear stockpile stewardship

What kinds of questions can mathematics help answer?

- Can we predict the operating characteristics of a clean coal power plant?
- How stable is the plasma containment in a Tokamak?
- How quickly is climate change occurring and what are the uncertainties in the predicted time scales?
- How quickly can an introduced bio-weapon contaminate the agricultural environment in the US?
- How do we modify models of the atmosphere and clouds to incorporate newly collected data (possibly of new types)
- How quickly can the US recover if part of the power grid became inoperable?
- What are optimal locations and communication protocols for sensing devices in a remote-sensing network?
- How can new materials be designed with a specified desirable set of properties?

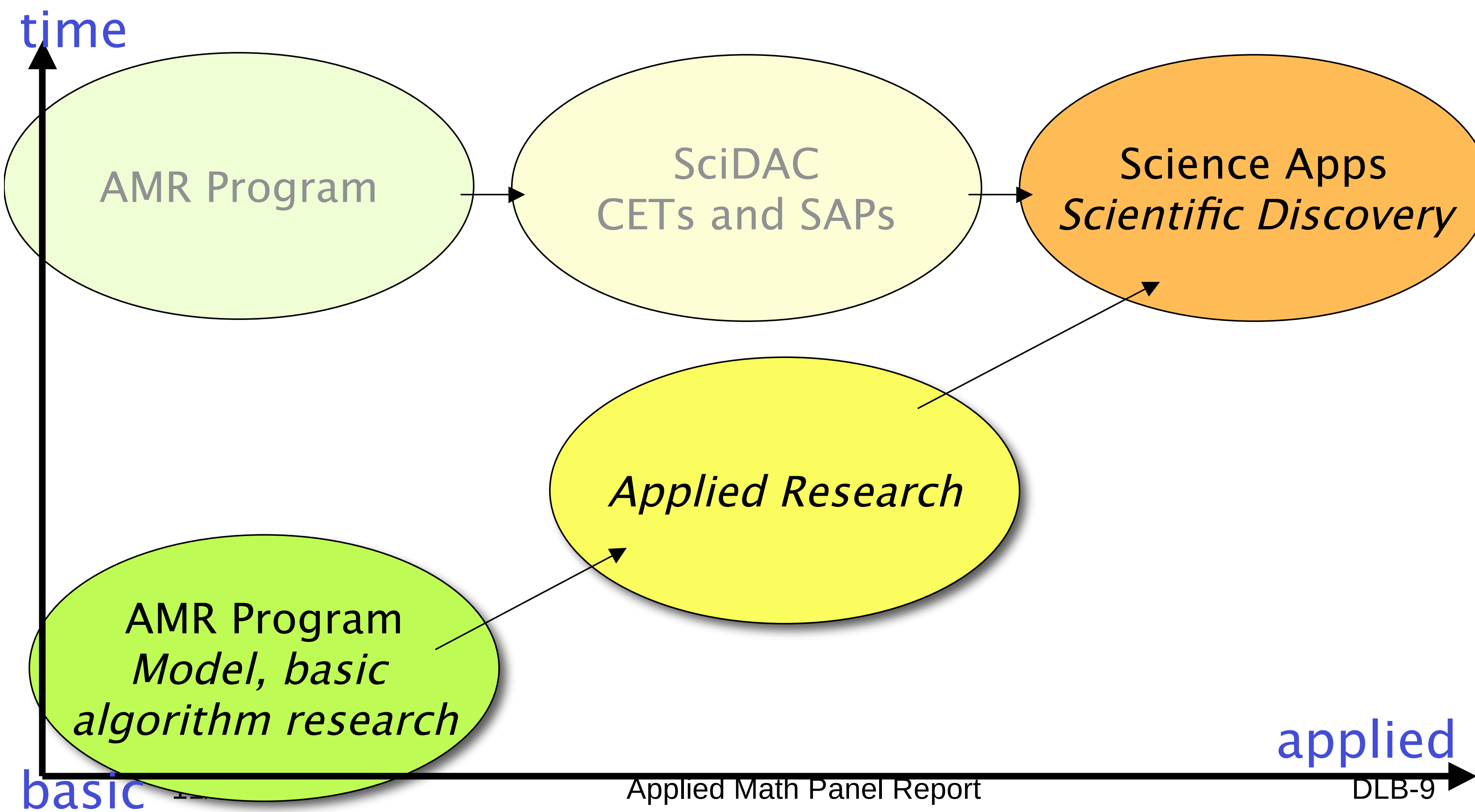
The questions asked are not necessarily answered by a single simulation



Mathematicians must learn to ask the right questions!

Need to understand the behavior of complex systems over ranges of parameter space

Advancing the mathematics of complex systems will require early collaboration with experts from other fields



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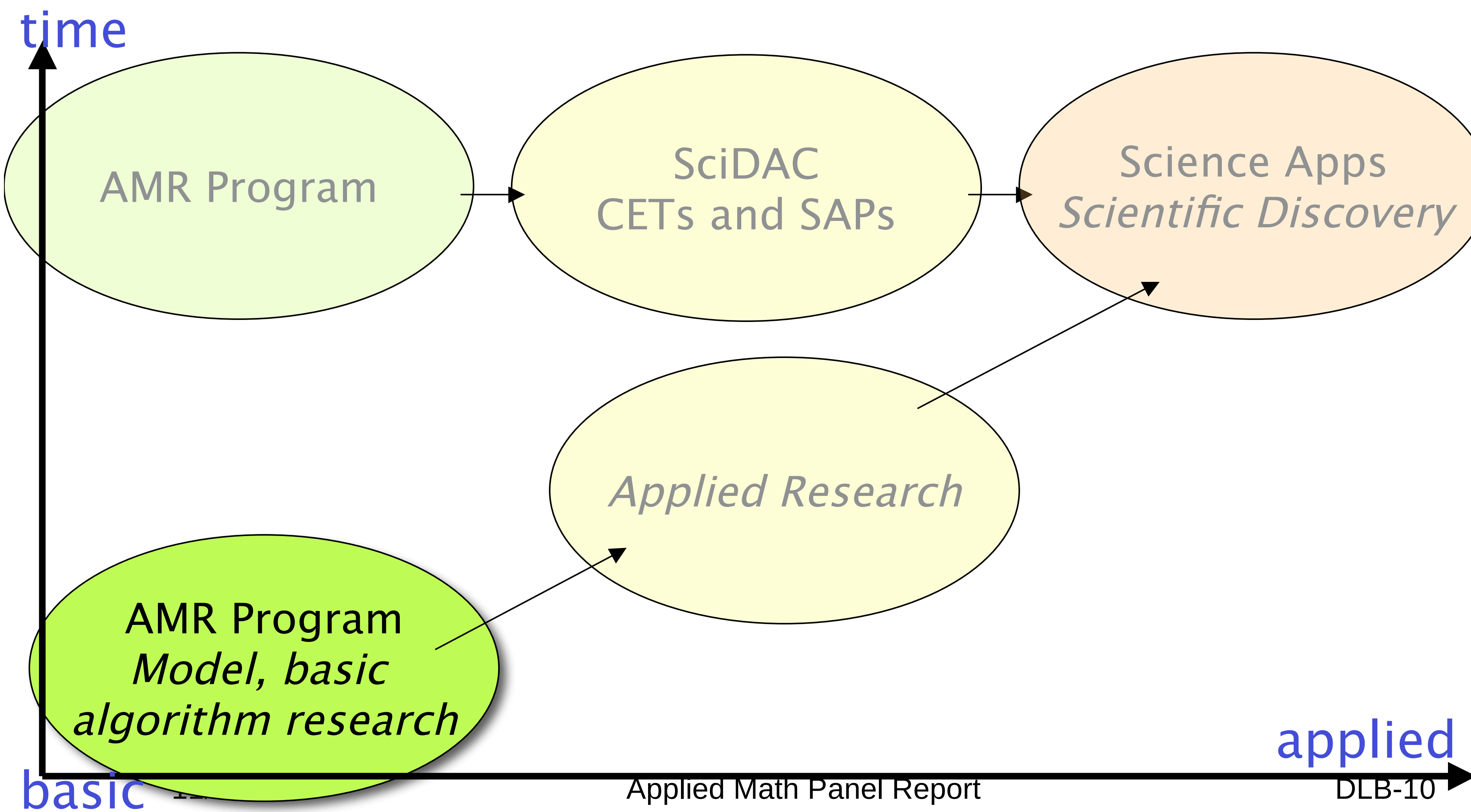


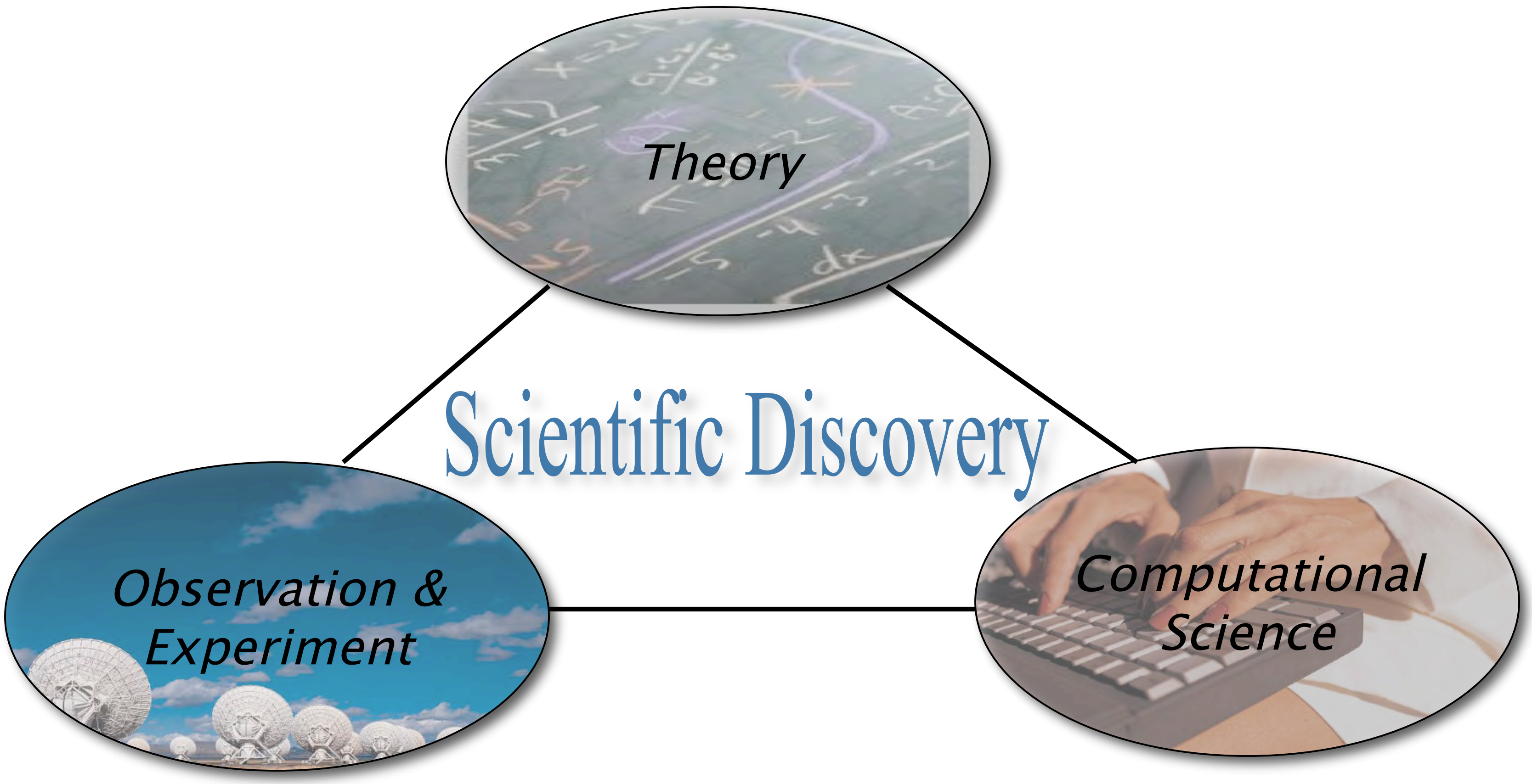
What are the mathematical characteristics of a complex system?

- A complex system is a collection of multiple processes, entities or nested subsystems where the overall system is difficult to understand and analyze because:
  - Components may have different mathematical structures, involve different temporal and spatial scales
  - Number of components can be very large
  - Connections in a variety of ways, often nonlinear
  - Taken collectively, the components form a whole whose behavior can evolve along qualitatively different pathways that may display great sensitivity to small perturbations at any stage *

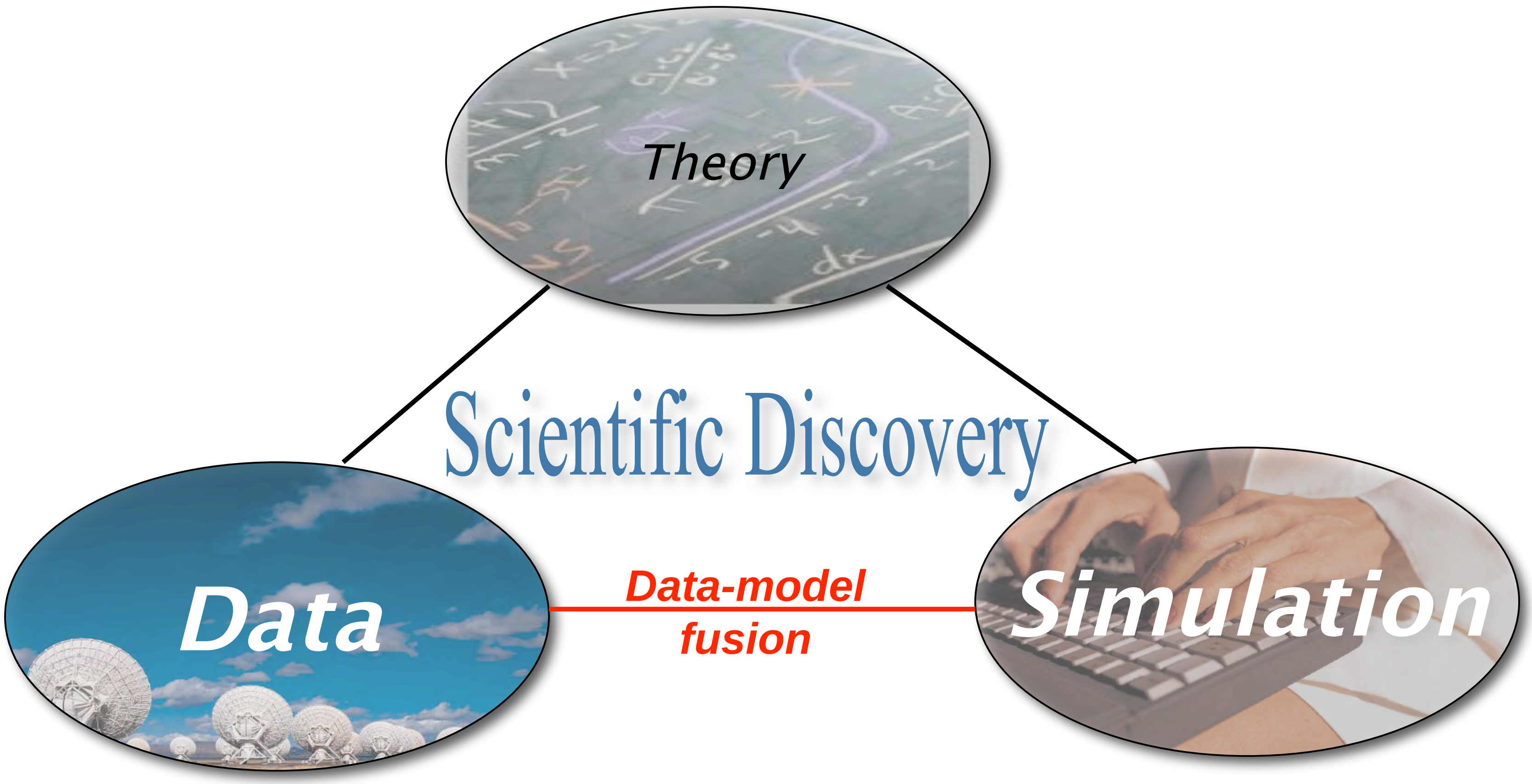
Classical reductionist approaches can totally miss significantly important behavior that arises due to combination of components in nonlinear ways

** Hendrickson & Wright, Optimization of Complex Systems Workshop Report, 2006*

Theory, experiment and computing will be required to understand complex systems



The mathematics involved in integrating data and simulation is increasingly important



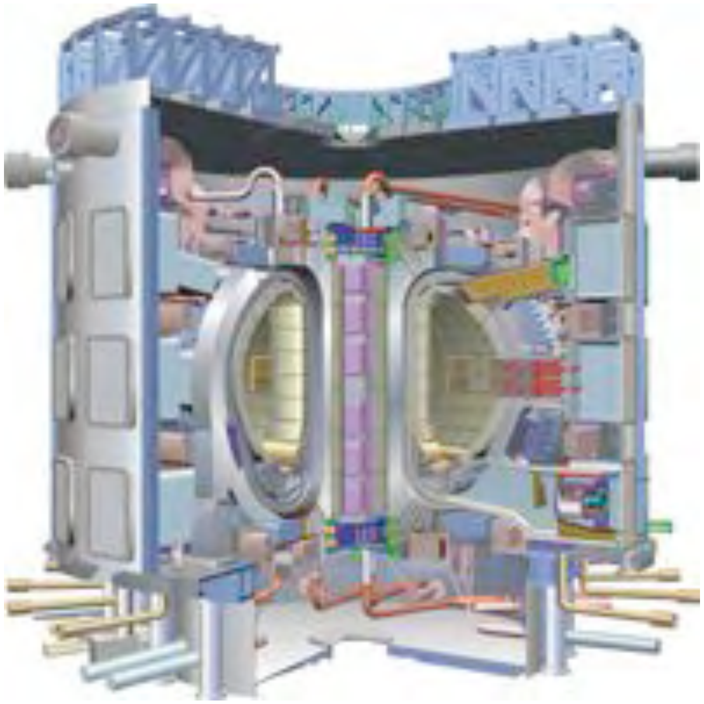
Data-model fusion is an essential element in understanding complex systems

- Neither experimental observation or mathematical and computational modeling alone can access all components of a complex system

- Three ways that models and data can be integrated:
  - *Empirical predictive models based entirely on data*
  - *Predictions based on physics-based math models, e.g. EOS, constitutive relations*
  - *Data assimilation*

Based on DOE mission needs, we identified mathematical challenges and approaches

- What are the types of questions that can be answered?
- What is the current state of the art?
- What are the outstanding research issues?
- What are strategies (research approaches) that will lead to the advancement of mathematics in this area?



We grouped the mathematical opportunities into three categories:

- Predictive modeling and simulation of complex systems
  - Advance the fidelity, predictability and sophistication of modeling and simulation methodologies for complex systems
- Mathematical analysis of the behavior of complex systems
  - Address the challenges of analyzing and understanding the behavior of math models for complex scientific and engineering systems
- Using models of complex systems to support decision making
  - Develop the math needed to support decision-making based on the prediction, optimization and understanding of complex systems

Predictive modeling and simulation of complex systems

- Multiscale, multiphysics and complex hybrid models
  - *Develop analytical and computational approaches needed to understand and model the behavior of complex multiphysics, and multiscale phenomena*
- The role of data-model fusion
  - *Enhance the theory and tools for complex multiscale, multicomponent models when observational or experimental data are incorporated in an essential way*
- Modeling stochastic effects in complex systems
  - *Develop new approaches for efficient modeling of large stochastic systems*
- Networks, Systems and Systems of Systems
  - *Develop mathematical techniques for decomposing complex systems into systems of canonical subsystems and modeling their behavior*

Mathematical analysis of the behavior of complex systems

- The role of data in the analysis and understanding of complex systems
  - *Develop sound, computationally feasible strategies and methods for the collection, organization, statistical analysis and use of data associated with complex systems*

- Sensitivity analysis
  - *Advance the theory and tools for sensitivity analysis to address the challenges posed by complex multiscale, multicomponent models*

- Uncertainty quantification and mitigation
  - *Significantly advance the theory and tools for quantifying the effects of uncertainty and numerical simulation error on predictions using complex models and when fitting complex models to observations*

Using models of complex systems to support decision making

- Mathematics of Risk analysis
  - *Significantly advance the math that supports risk analysis techniques for decision making about complex systems that include natural and engineered components, and economic, security and policy consequences*

- Optimization
  - *Develop techniques for formulating, analyzing and solving challenging optimization problems arising in complex natural and engineered systems*

- Inverse problems
  - *Develop techniques for addressing the mathematical and computational difficulties of inverse problems associated with complex systems*

Example: Develop analytical and computational approaches needed to understand and model the behavior of complex phenomena

- Strategies to accomplish this goal:

We are developing strategies for each goal

  - Develop analytical tools for decomposing complex, multiphysics systems into their component processes and for elucidating the coupling between these component pieces;
  - Develop methodologies for representing behavior at fine scales in models for the system at larger scales. Develop the corresponding analytical tools and computational approaches needed to quantify the impact of the fidelity of finer-scale models on large-scale dynamics;
  - Develop algorithmic techniques for simulating multiphysics and multiscale processes with quantifiable fidelity;
  - Develop and analyze numerical methods for hybrid models that couple continuum and discrete processes. How do changes in the discrete variables affect the accuracy of the continuum part of the model?
  - Develop approaches for deriving computationally tractable approximations to systems that are formulated in very high dimensional spaces, such as those arising in quantum mechanics.

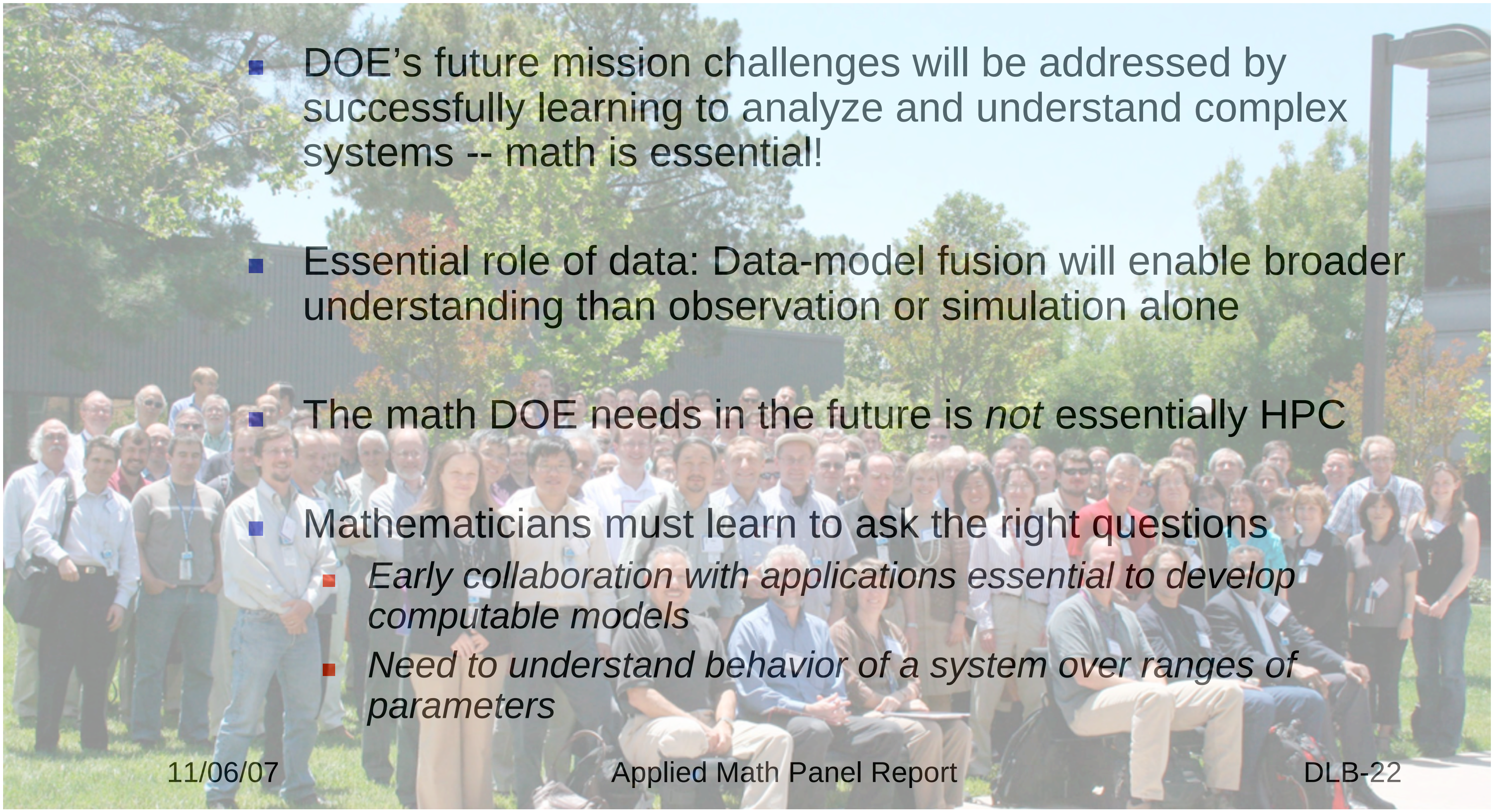
Many of the mathematical challenges are not HPC in nature, and may not result in research activities involving HPC

The mathematics for complex systems will build on the strong foundations of the AMR program

- Linear and nonlinear equations
- Numerical methods for differential equations
- Computational geometry
- Optimization methods
- Fast graph algorithms
- Fast algorithms for continuous and N-body problems
- Reduced-order modeling
- Dynamical systems theory
- HPC as an enabling technology

These are not "finished" products "reduced to practice", but frameworks for attacking new problems

There is a rich future for applied and computational mathematics in the DOE



- DOE's future mission challenges will be addressed by successfully learning to analyze and understand complex systems -- math is essential!
- Essential role of data: Data-model fusion will enable broader understanding than observation or simulation alone
- The math DOE needs in the future is *not* essentially HPC
- Mathematicians must learn to ask the right questions
  - *Early collaboration with applications essential to develop computable models*
  - *Need to understand behavior of a system over ranges of parameters*